The NAVY/NASA Engine Program (NNEP89)— Interfacing the Program for the Calculation of Complex Chemical Equilibrium Compositions (CEC)

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CONTENTS

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SUMMARY

The Navy/NASA Engine Program - NNEP, is a general computer program for calculating aircraft engine performance. NNEP has been used extensively to calculate the design and off-design (matched) performance of a broad range of turbine engines, ranging from subsonic turboprops to variable cycle engines for supersonic transports. Recently, however, there has been increased interest in applications for which NNEP is not capable of simulating, such as the use of alternate fuels including cryogenic fuels and the inclusion of chemical dissociation effects at high temperatures. To overcome these limitations, NNEP has now been extended by including a general chemical equilibrium method. This permits consideration of any propellant system and the calculation of performance with dissociation effects. The new extended program is referred to as NNEP89.

INTRODUCTION

The Navy/NASA Engine Program - NNEP, is a general computer program for calculating aircraft engine performance and is described in references 1-4. NNEP has been used extensively to calculate the design and off-design (matched) performance of a broad range of turbine engines, ranging from subsonic turboprops to variable cycle engines for supersonic transports. The NNEP computer code has gained wide acceptance and is currently in use at over 70 universities, commercial companies and other government agencies. Recently, however, there has been increased interest in applications for which NNEP is not capable of simulating, such as the use of alternate fuels including cryogenic fuels and the inclusion of chemical dissociation effects at high temperatures. To overcome these limitations, NNEP has now been extended by including the general equilibrium method of reference 5 (referred to here as CET86). This permits consideration of any propellant system and the calculation of performance with dissociation effects. The new extended program described herein will be referred to as NNEP89.

Inasmuch as the option of obtaining performance based on no dissociation is still available, all of the subroutines in NNEP have been retained, but with appropriate revisions to accommodate the new dissociation option in NNEP89. Many of the subroutines in CET86 were eliminated (such as those pertaining to shock and detonations) and changes were made in a number of the remaining subroutines to join CET86 with NNEP. In addition, two new subroutines were prepared: GASGEN and THERME. Subroutine GASGEN extends the modelling capabilities of NNEP by permitting the burning of energetic combinations such as hydrogen and oxygen or methane and oxygen in a gas generator. Subroutine THERME was prepared to replace function THERM when thermodynamic properties of dissociated mixtures are required.

This report presents information on input and output which is required in addition to the information already presented in references 4 and 5; a description of some of the changes or additions to several subroutines; and a few sample problems. For the user of this program, the principal new information concerning input preparation is discussed in several sections under "INPUT INSTRUCTIONS". Additional input information for the gas generator is given in the section "Subroutine GASGEN". The other sections, which are primarily concerned with changes or additions to some of the routines from the NNEP or CET86 programs, are not necessary for using the program but are included for the sake of completeness.

INPUT INSTRUCTIONS

Options for Running With or Without Dissociation

No changes in input are required if NNEP89 is to run as NNEP was previously, i.e., if engine performance without chemical dissociation is desired. To obtain performance with dissociation, three additional types of input are required. The first simply requires the index ICEC to be set equal to 1 in the first &D namelist. If ICEC=1, then subroutine MAINEQ is called from

subroutine INPUT to initiate all the preparation that is required for chemical equilibrium calculations such as reading in the REACTANT information and the appropriate thermodynamic data. The second type of input requires the preparation of REACTANT card images similar to those discussed in reference 5. Changes that were made in the reference 5 format for REACTANTS are discussed in the next section. The third type of input involves the arrays FARRAY and OARRAY which are discussed in a later section. If a run is to be made involving the gas generator, then some additional input is required in the SPEC array for the generator. The details of this input are discussed in the section "Subroutine GASGEN".

In addition to the required types of input, some optional input variables have been provided for debugging purposes (see section "Debugging").

REACTANT Card Images

As mentioned previously, REACTANT card images are required for the option of chemical dissociation. A maximum of 24 reactants is permitted for any computer run. The first reactant must always be air. The format for these card images, presented in reference 5, has been changed somewhat for this program. The revised format is given in Table 1. The revisions permit the option of specifying for each reactant either an assigned enthalpy (as discussed in reference 5) or a heat of combustion. Two energy units are currently permitted for the assigned enthalpy: calories or joules. The heat of combustion is in units of BTU/lb. The units for the energy value given in columns 54-62 are now indicated by the index in column 71 as follows:

Column 71	Columns 54-62
Blank	Enthalpy in units of cal/formula weight
J	Enthalpy in units of joules/formula weight
B	Heat of combustion in units of BTU/lb

Heat of combustion may be specified as the lower heating value (LHV) or the higher heating value (HHV). (The LHV is the heat of combustion value when the combustion product H_2O is in the gaseous state, whereas for the HHV value the H_2O is in the liquid state.) To specify the HHV, the heat of combustion value in card columns 54-62 must be put in as a negative number. Otherwise, the program assumes it is the LHV. Columns 73-80 are used for combustion efficiency. These columns are used only in conjunction with the heat of combustion. If columns 73-80 are blank for a given heat of combustion, a default value of 1 is used by the program. The heat of combustion and efficiency are automatically converted in the program to an equivalent assigned enthalpy value as required by the chemical equilibrium routines. A reactant may also be one of the possible products of combustion included in the set of thermodynamic data used in NNEP89 (see section THERMODYNAMIC DATA). When this occurs, the program provides an option for automatically calculating the enthalpy of the reactant at the temperature specified in columns 64-70. This is accomplished by putting zeros in columns 37 and 38. In reference 5,

the REACTANT card image uses columns 46-53 to specify the relative weight of the reactant. In NNEP89 these columns are not used, inasmuch as relative weights of reactants are specified by the arrays FARRAY and OARRAY (see discussion in next section). Temperature, in units of kelvin, is restricted to columns 64-70. In reference 5, temperature is given in columns 64-71. If zeros are put in columns 37 and 38 for some reactant as discussed above, then a temperature in columns 64-70 is required. Otherwise, temperature in these columns is optional and may be omitted or included for informational purposes only. Also, in reference 5, a reactant is identified as a fuel or as an oxidant by an "F" or "O" in column 72. This is no longer required in NNEP89 but may be used for informational purposes. As each REACTANT card image is read, NNEP89 automatically assigns it a number in the order it is read. This reactant order number is required by the user for the preparation of the FARRAY and OARRAY arrays (see next section).

FARRAY and OARRAY

Only one fuel can be specified in NNEP for any particular run. The arrays FARRAY (12,200) and OARRAY (12,200) are part of the arrangement for making NNEP89 completely general in regard to the number and type of reactants which can be considered and for specifying which reactants are to be added to which engine component. At present, the FARRAY is used only for burners and gas generators while the OARRAY is used only for gas generators. FARRAY is used for fuels and OARRAY for oxidants. The first index, with dimension 12, is used to specify from 1 to 6 pairs of numbers. The first number of each pair is the reactant order number (see section Subroutine REACT) and the second number of each pair is its weight relative to the total weight of reactants being added to the engine component specified by the second index. If only one reactant is added to a particular component, its relative weight is 1. The second index, with dimension 200, specifies the engine component number. The FARRAY may be used with or without the OARRAY. Some examples will help to clarify the use of these arrays.

Example 1. In this simple case, just one fuel, REACTANT 2, with a relative weight fraction of 1., is being added to the burner, which, in this example, is component 3. Then FARRAY(1,3)=2 and FARRAY(2,3)=1. The same information is specified by setting FARRAY(1,3)=2,1.

Example 2. Two fuels are being added to the burner, component 5. These fuels are REACTANT 2 with a weight fraction of 0.4 and REACTANT 3 with a weight fraction of 0.6. Then FARRAY(1,5)=2,.4,3,.6

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Example 3. The burner is component 6, using REACTANT 2 fuel. In addition, REACTANT 3 (a fuel) and REACTANT 4 (an oxidant) are being added to the gas generator, engine component 5. Then

For the burner: FARRAY(1,6)=2,1.

For the gas generator: FARRAY(1,5)=3,1 and OARRAY(1,5)=4,1.

Debugging

The CET86 program provides for debugging with the index IDEBUG. Setting IDEBUG to some value other than zero gives intermediate output that is useful, for example, for finding programming errors, studying the iteration process and rate of convergence for obtaining chemical equilibrium, and for verifying that thermodynamic data have been properly prepared. Some discretion should be exercised in connection with using IDEBUG inasmuch as this option can generate an enormous amount of intermediate output in the NNEP89 program (as much as a factor of 100 compared to the standard output). It is generally preferable to use the CET86 program for this type of debugging. Additional debugging capabilities have been provided in NNEP89 by use of indices IDBUG, LDBUG, and NDBUG. All four debugging controls are part of namelist &INPT2. The default value for these controls is zero. At present, the following intermediate output is obtained for the following values of IDBUG:

Value of IDBUG	Intermediate Output	
1	1.	Name of the subroutine being called from among the following subroutines: COMPRS, DBURNR, GASGEN, HEATXC, INLET, MIXER, NOZZLE, SPLITR, and TURBIN
	2.	Values of JCX, JM1, JM2, JP1, JP2 for current subroutine. (from among the above subroutines) (Also values of IWAY and IDONE for subroutine INLET)
2	1.	The output for IDBUG = 1
	2.	Values of PECWT (see "Defining the Chemical System")
	3.	Value of stoichiometric f/a in DBURNR subroutine

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| 3 | 1. | The output for IDBUG = 2 |
| | 2. | Details of convergence procedures for subroutines DBURNR and GASGEN |

Value of LDBUG

| 1 | 1. | Details of convergence procedures for subroutine THERME (ID=8) (See "Subroutine THERME" for definition of ID) |

Value of NDBUG

| 1 | 1. | Details of convergence procedures for subroutine THERME (ID=1,2,3 and 7) |

An example of input containing a debug parameter is shown in APPENDIX B (TESTCASE: SEPARATE FLOW TURBOFAN).

DESCRIPTION OF SUBROUTINES

Defining the Chemical System

Several subroutines and COMMON regions are involved in defining a current chemical system. The region WTREAC(24,100) contains the flow rates of up to 24 reactants (first index) for each of up to 100 flow stations (second index). At the beginning of each subroutine that requires thermodynamic properties of the flow, the flow rates from the immediately upstream component are read from WTREAC and stored in region PECWT(24). In most subroutines, the incoming flow remains unchanged. However, in several subroutines, additional reactants may be added to the incoming flow. These additional reactants and their relative amounts by weight are specified by information in FARRAY and OARRAY (see section FARRAY and OARRAY). In those subroutines where the values of PECWT change due to the addition of reactants, the new values of PECWT are stored in WTREAC.

When additional reactants are added, a new chemical system is automatically set up by NNEP89 for the equilibrium calculations. This is accomplished by 1) calling subroutine REACT (which searches the reactants for all chemical elements in the system); 2) calling SEARCH (to select all possible chemical species in the system that are contained in the thermodynamic library) and 3) setting NEWFA=1. When NEWFA=1, subroutine THERME will call NEWOF to set up new relative atom ratios (kg-atoms/kg) for the chemical elements.

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Subroutine DBURNR

An iterative procedure is required to find the f/a (fuel-to-air weight ratio) corresponding to an assigned burner-out temperature. Note that "fuel" in the f/a ratio includes any reactant that is carried on board including oxygen as well as jet fuel, hydrogen, etc. For the no dissociation option, the iterative procedure described in reference NNEP was not changed. However, for the dissociation option, a different procedure is used and is described as follows. A chemical equilibrium calculation for any f/a at the burner-out temperature permits obtaining a corresponding value of Δh defined as

$$\Delta h = H_p - H_r \tag{1}$$

where H_p is the enthalpy of the products at the assigned burner-out temperature reaction and H_r is the enthalpy of the mixture of reactants. The correct value for f/a is obtained when $\Delta h = 0$. The iteration procedure consists of setting up a linear equation for two values of f/a and their corresponding Δh values and solving for an improved value of f/a by setting $\Delta h = 0$ in the linear equation

$$f/a = m\Delta h + b \tag{2}$$

where

$$m = ((f/a)_2 - (f/a)_1)/(\Delta h_2 - \Delta h_1) \tag{3a}$$

and

$$b = (f/a)_2 - m\Delta h_2 \tag{3b}$$

This improved value of f/a and its corresponding value Δh are used together with one of the two previous sets of f/a's and Δh's to obtain an even closer value of f/a by again using equations (2), (3a) and (3b). This procedure is repeated until convergence is reached as defined by the following equation:

$$|\ ((f/a)_2 - (f/a)_1)/(f/a)_1\ |\ \leq 0.000005 \tag{4}$$

Initial estimates for two values of f/a are required to start the iteration process. However, except for $(f/a)_s$ (the stoichiometric condition), f/a is a double-valued function of burner-out temperature. That is, the same burner-out temperature can be obtained by burning lean or rich. Therefore, different sets of initial estimates for f/a are required for the lean or rich side of stoichiometric. The specification of whether the burner is to burn lean, rich or stoichiometric is accomplished by setting SPEC (11,N) as follows (where N is the number of the burner component):

Burn condition	Value of SPEC (11,N)
lean	0
stoichiometric	1
rich	2

If SPEC (11,N)=1, no iteration for f/a is required inasmuch as (f/a)s is known from a previous calculation.

If SPEC (11,N)=0 (lean), the two initial estimates for f/a are obtained as follows. One of these estimates is obtained by means of the equation.

$$(f/a)_1 = (-2.2085 \times 10^{-3} - 8.1876 \times 10^{-6} T_i) + \tag{5a}$$

$$(1.3595 \times 10^{-5} - 4.77162 \times 10^{-9} T_i) T_e +$$

$$(1.21147 \times 10^{-9} + 7.2503 \times 10^{-13} T_i) T_e^2 + (f/a)_i$$

where T_i is the incoming temperature in °R, T_e is the assigned burner exit temperature in °R and $(f/a)_i$ is the value of the incoming fuel/air ratio. Equation (5) was obtained by fitting results for a hydrocarbon with an H/C atom ratio of 1.917, a heat of combustion of 18,300 BTU/lb and a combustion efficiency of 0.995; a range of inlet air temperatures from 540 to 1620 °R; and a range of exit temperatures from 540 to 4500 °R. The second initial estimate for f/a is simply the value obtained from equation (5) plus 0.01, i.e,

$$(f/a)_2 = (f/a)_1 + 0.01 \tag{5b}$$

If SPEC (11,N) = 2 (rich), the two initial estimates for f/a are obtained as follows:

If $(f/a)_i < (f/a)_s$, then

$$(f/a)_1 = (f/a)_s + 0.01 \tag{6}$$

If $f/a_i > (f/a)_s$, the

$$(f/a)_1 = (f/a)_i + 0.01 \tag{7}$$

In either of the above cases

$$(f/a)_2 = (f/a)_1 - 0.002 \tag{8}$$

Subroutine GASGEN

Subroutine GASGEN calculates the combustion properties of reactants in a gas generator. The REACTANT data for the gas generator are read in together with REACTANT data for other components (see section REACTANT Card Images). The specifications for generator operating conditions are given on the GGEN SPEC card image in the NNEP input. The inputs and outputs for the gas generator are as follows:

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INPUTS

[a]SPEC(1,N)=assigned exit temperature, °R

[a]SPEC(2,N)=fuel/oxidant weight ratio

SPEC(3,N)=generator pressure, psia (used only if zero flow into gas generator)

[a]SPEC(4,N)=fuel flow rate, lb/sec

[a]SPEC(5,N)=oxidant flow rate, lb/sec

[a]Not all of these SPEC's can be specified simultaneously. The options are:

     1.   SPEC(1,N) and SPEC(4,N)

     2.   SPEC(1,N) and SPEC(5,N)

     3.   SPEC(2,N) and SPEC(4,N)

     4.   SPEC(2,N) and SPEC(5,N)

     5.   SPEC(4,N) and SPEC(5,N)

OUTPUTS

DATAOUT(1,N) -generator temperature, °R

DATAOUT(2,N) -assigned generator f/o ratio

DATAOUT(3,N) -generator pressure, psia

DATAOUT(4,N) -generator fuel flow rate, lb/sec

DATAOUT(5,N) -generator oxidant flow rate, lb/sec

DATAOUT(6,N) -total generator flow rate, lb/hr

DATAOUT(7,N) -calculated generator f/o ratio for assigned exit temperature

If the generator exit temperature is assigned (input options 1 or 2 above), the f/o ratio is determined by an iterative process similar to that described for obtaining f/a in subroutine DBURNR. In general, the f/o ratio is a double-valued function of temperature corresponding to the lean and rich side of stoichiometric. Therefore, if temperature is assigned, it is necessary to start with an estimate of f/o on the side of stoichiometric that is desired. At present the program defaults to an f/o value of 0.3 which is on the rich side of stoichiometric for H_2-O_2 and CH_4-O_2. If an initial estimate different from 0.3 is desired, it can be specified with SPEC(2,N). (Note that if SPEC(2,N) is specified together with option 1 or 2 above, then SPEC(2,N) is used only as an initial estimate for f/o and not as a final assigned value.)

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In addition to the new subroutine GASGEN, some program changes were required in other subroutines to accommodate engine designs which include a gas generator. These changes are either used or bypassed according to whether the logical word GNRATR is either TRUE or FALSE. The default value of GNRATR is FALSE and is set equal to TRUE in subroutine GASGEN.

Subroutine MIXER

This subroutine was modified for chemical equilibrium purposes by permitting two propellant streams with possibly different chemical systems to be combined into one overall chemical system. The procedure for accomplishing this is explained in the section "Defining the Chemical System".

Subroutine NEWOF

Subroutine NEWOF combines individual values of HPP(N) (enthalpy of reactant N) and BOP(J,N) (atoms of chemical element J per gram of reactant N) into an overall chemical system value of HSUBO (enthalpy per gram of mixture) and set of BO(J) (atoms of chemical element J per gram of mixture). The values of HPP(N) and BOP(J,N) have previously been calculated and stored in subroutine REACT. They are combined in proportion to the current set of flow rates of the individual reactants PECWT(N). Subroutine NEWOF is required to be called only when the values in PECWT(N) have changed. The program automatically takes care of this.

Subroutine REACT

The CET86 version of Subroutine REACT was modified for NNEP89. The purpose of this modification was to permit the chemical system to be changed at different points in the engine cycle. REACT is initially called from MAINEQ for the purpose of reading and storing the input information contained in the REACTANT card images (see section "REACTANT Card Images"). A maximum of 24 reactants is permitted. The first reactant must always be air. For each chemical element J in each reactant N, the atoms per gram of reactant are calculated and stored in region BOP(J,N). Reactant energies may be either in the form of an assigned enthalpy or heat of combustion (see section "REACTANT Card Images"). If a heat of combustion is given, subroutine REACT converts it to an assigned enthalpy relative to a selected enthalpy base (see section "THERMODYNAMIC DATA"). Enthalpies of the individual reactants are stored in HPP(N). The values of HPP(N) and BOP(J,N) are combined in subroutine NEWOF to obtain an overall enthalpy HSUBO and set of BO(J) for the current chemical system. After the initial call from MAINEQ, subroutine REACT may be called from any of a number of subroutines when the chemical system is to be changed. These subroutines are COMP, COOLIT, DBURNR, GASGEN, HTEX, INLET, MIXER, NOZZLE, and TURBIN. Subroutine REACT also calculates the stoichiometric f/a ratio for the current chemical system in subroutine DBURNR.

Subroutine SETEN

Chemical equilibrium compositions are obtained by an iteration process which requires an initial estimate of compositions. On the first pass of the engine cycle, arbitrary initial estimates of compositions are used in some of the engine components. Once converged compositions have been obtained in the first pass, considerable computer time can be saved by not repeating the iteration process in subsequenent passes. This is accomplished by using subroutine SETEN to save converged compositions from each pass to use in subsequent passes where applicable. Provision has been made to save compositions for each engine component, where needed, inasmuch as the chemical system may change from component to component. Saving and restoring compositions are accomplished automatically in the program by means of the index ISV. Before calling SETEN, setting ISV= -1 saves compositions, whereas setting ISV= 0 restores compositions.

Subroutine THERME

In the NNEP program, thermodynamic mixture properties are obtained by means of the function THERM(ID,ARG,FAOLD,DUMMYP), where ID is an index indicating which dependent function is desired, ARG is the value of the independent function, FAOLD is the f/a value and DUMMYP is the value of pressure. A separate statement is required for each function desired, such as enthalpy, relative pressure ratio, ratio of specific heats, and universal gas constant divided by molecular weight. Six ID's are contained in THERM as shown in Table 2. For the dissociation option in NNEP89, the thermodynamic mixture properties are obtained by means of a new subroutine THERME(ID,ARG,FAOLD,DUMMYP), where the vector parameters are the same as in function THERM. There are some similarities and some differences between THERM and THERME. One difference, for example, is in the number of thermodynamic state functions which need to be specified. In general, a thermodynamic state is defined by specifying two independent state functions such as temperature and pressure or enthalpy and pressure. This is what is required by THERME to obtain equilibrium mixture properties. However, when no chemical dissociation occurs, thermodynamic properties are independent of pressure, and therefore any value may be used in the function THERM for DUMMYP (hence the name). In THERME, once the chemical equilibrium compositions have been determined, then all the dependent state functions and thermodynamic properties and derivatives can be calculated. Therefore, some of the ID's in THERM (ID's 5 and 6) are no longer necessary in THERME. In addition, ID equal 7 and 8 were added in THERME. ID=7 is used for an assigned enthalpy-entropy problem while ID=8 is used for an assigned Mach number problem. The parameter FAOLD is always the fuel/air ratio in both THERM and THERME. Table 3 lists the possible ID's in THERME. As pointed out in the next section, a different set of units is used in the NNEP subroutines and in the subroutines taken from CET86. The transfer between the two sets of units is handled in subroutine THERME.

THERMODYNAMIC DATA

The thermodynamic data and enthalpy base are not the same for NNEP and for NNEP89. The thermodynamic data for NNEP are based on the data given in reference 6. Mixture properties in reference 6 do not include effects of dissociation, and therefore the only species considered are CO2, H_2O, N_2, O_2, and Ar. The enthalpy base in reference 6 is 0 at a temperature of 0 K. In NNEP89, the following 20 species are considered as possible products of combustion for the C, H, O, N, Ar chemical system: Ar, CH_2, CH_4, CO, CO_2, H, HO_2, H_2, H_2O, $H_2O(1)$, H_2O_2, N, NH_3, NO, NO_2, N_2, N_2O, O, OH, and O_2. Thermodynamic data and heats of formation are taken from reference 7 for all the previous species except for NO, NO_2 and N_2O which were taken from reference 8. The enthalpy base for species in NNEP89 is 0 at 298.15 K for C (graphite), H_2, O_2, N_2 and Ar. For each of the other species, the enthalpy value at 298.15 K is its heat of formation at 298.15 K relative to the previous five base species. The thermodynamic data have been reduced to functional form by means of a least squares fit as discussed in reference 5. The least squares coefficients that are used to reproduce the thermodynamic data are stored by subroutine UTHERM in unformatted form. The NNEP subroutines use thermodynamic properties in U.S. customary units (for example: enthalpy in BTU/lb, temperature in °R and pressure in psia). The CET86 subroutines use thermodynamic properties in the following units: enthalpy in cal/gm, temperature in kelvin and pressure in atmospheres. The transfer from one set of units to the other is handled in subroutine THERME.

In addition to the previously discussed species, several "fictitious" species are also included. These will be referred to as inert species; namely, inert H (IH), inert H_2 (IH_2), inert CH_2 ($ICIH_2$) and inert CH_4 ($ICIH_4$). These inert species are formed from fictitious "inert chemical elements" IC and IH. The inert species have the identical thermodynamic properties as their corresponding conventional species (H, H_2, CH_2 and CH_4). The purpose for including these inert species is to provide a technique for simulating incomplete combustion of fuels. For example, say it is desired to use H_2 as a fuel and to calculate the results for only 85 percent complete combustion. This can be accomplished by using two reactant cards for hydrogen - one containing H_2 and the other containing IH_2. If H_2 were reactant 3 and IH_2 were reactant 4 and the component using them were 5, then the FARRAY for that system would be FARRAY(1,5)=3,.85,4,.15. The program would then permit the 0.85 fraction of H_2 to burn and produce whatever combustion products result from the chemical equilibrium calculations, but the 0.15 fraction of IH_2 would produce only IH_2 and IH as products. The same technique can be used for any hydrocarbon fuel. For example, in addition to a reactant card for a fuel with an empirical formula $CH_{.524504}$ one would also include a reactant card with the formula $ICIH_{.524504}$. The relative fractions of these fuels would again be specified by an appropriate FARRAY. In this case, in addition to the usual combustion products, all four of the fictitious inert species would be considered during the equilibrium calculations. In order to use this inert species technique to simulate partial combustion, it was necessary to include the "inert elements" IC and IH in BLOCK DATA. The data in BLOCK DATA for elements IC and IH are identical to that for C and H respectively.

APPENDIX A

SYMBOLS

b	coefficient in eq. 2 (defined in eq. 3b)
B	symbol used on REACTANT card image to indicate heat of combustion
BO(I)	kg-atoms of chemical element I per kg of mixture
BOP(I,N)	kg-atoms of chemical element I per kg of reactant N
f/a	fuel-to-air weight ratio
f/o	fuel-to-oxidant weight ratio
H	enthalpy
H/C	hydrogen-to-carbon atom ratio
HHV	higher heating value (higher heat of combustion)
ICEC	index to obtain performance based on dissociation (ICEC = 1) or no dissociation (ICEC = 0)
IDBUG	index for debugging (see discussion p.7)
ISV	index for saving compositions (ISV = -1) or restoring compositions (ISV = 0)
J	symbol used on REACTANT card image to indicate enthalpy in joules
LDBUG	index for debugging (see discussion p.7)
LHV	lower heating value (lower heat of combustion)
m	slope (eqs. 2 and 3a)
NDBUG	index for debugging (see discussion p.7)
PECWT(N)	flow rate of reactant N, lb/sec
R/M	universal gas constant divided by molecular weight
T	temperature

WTREAC(N,J) flow rate of reactant N in flow station J, lb/sec

Δh   difference between enthalpy of reactants and enthalpy of products, eq. 1

&D   namelist D

&INPT2   namelist INPT2

APPENDIX B

SAMPLE PROBLEMS

```
TEST CASE:  MIXED FLOW TURBOFAN  SANFORD NEW
 &D ICEC=1, LONG=F, NCODE=1, DRAW=T, NMODES=1, &END
REACTANTS
N 1.5606  O 0.4198  AR .0098                    100.  0.0      G 298.15 O
C 0.5245  H 1.0000                              100. -4628.066L 298.15 F

END
 &D MODE=1,
 XNUM=4HINLT,4HLPCI,4HSPLI,4HHPCI,4HMBRN,4HHPTI,4HMXRI,
 4HABRN,4HNOZI,4HNOZO,4HSECI,4HSECO,
 KONFIG(1,1)=4HINLT,1,0,2,0,SPEC(1,1)=100.0,0.,0.,0.,0.,0.,0.,
 0.,0.,0.,0.,18.00,
 KONFIG(1,2)=4HCOMP,2,0,3,0,SPEC(1,2)=1.60,0.,1,1001,1,1002,1,
 1003,1,0.,0.,0.84,2.9,0.95,
 KONFIG(1,3)=4HSPLT,3,0,4,12,SPEC(1,3)=1.75,0.02,0.02,
 KONFIG(1,4)=4HCOMP,4,0,5,0,SPEC(1,4)=1.30,0.,1.,1004,1,1005,1,
 1006,1,0.,0.,0.84,6.0,1,
 KONFIG(1,5)=4HDUCT,5,0,6,0,SPEC(1,5)=.05,0,0,3000.,.99,18300.,
 FARRAY(1,5)=2,1,
 KONFIG(1,6)=4HTURB,6,0,7,0,SPEC(1,6)=3.6,1.0,1,1007,1,1,1,1,1,1,
 .90,5000,1,
 KONFIG(1,7)=4HMIXR,7,13,8,0,SPEC(1,7)=0.,0.,0.40,1.,0.,0.,
 KONFIG(1,8)=4HDUCT,8,0,9,0,SPEC(1,8)=.05,0,0,3600.,.99,18300.,
 FARRAY(1,8)=2,1,
 KONFIG(1,9)=4HNOZZ,9,0,10,0,SPEC(1,9)=0.,0.98,0.,0.,.98,1.,1.,
 0.,1.,
 KONFIG(1,10)=4HDUCT,12,0,13,0,SPEC(1,10)=.05,0,0,0.,0.99,18300.,
 FARRAY(1,10)=2,1,
 KONFIG(1,11)=4HSHFT,2,4,6,0,SPEC(1,11)=9*1.0,
 KONFIG(1,12)=4HCNTL,SPCNTL(1,12)=1,1,4HSTAP,8,2,0,0,
 KONFIG(1,13)=4HCNTL,SPCNTL(1,13)=1,4,4HSTAP,8,4,0,0,
 KONFIG(1,14)=4HCNTL,SPCNTL(1,14)=1,11,4HDOUT,8,11,0,0,
 KONFIG(1,15)=4HCNTL,SPCNTL(1,15)=1,6,4HSTAP,8,6,0,0,
 KONFIG(1,16)=4HCNTL,SPCNTL(1,16)=1,3,4HDOUT,8,7,0,0,
 KONFIG(1,17)=4HCNTL,SPCNTL(1,17)=1,2,4HDOUT,5,2,50,0,
 &END
 &D SPEC(9,12)=1.0,SPEC(9,13)=1.0,SPEC(9,14)=1.0,SPEC(9,15)=1.0,
 SPEC(5,1)=.26,SPEC(9,1)=50,SPEC(6,1)=0,
 SPEC(9,16)=1.0,SPEC(9,17)=0.0,&END
 &D SPEC(5,1)=.6,SPEC(9,1)=10000,&END
 &D SPEC(5,1)=.9,SPEC(9,1)=25000,&END
 &D SPEC(5,1)=1.2,SPEC(9,1)=32200,&END
 &D SPEC(5,1)=1.5,SPEC(9,1)=39500,&END
 &D SPEC(5,1)=1.8,SPEC(9,1)=46800,SPEC(4,5)=3400,&END
 &D SPEC(5,1)=2.0,SPEC(9,1)=50900,SPEC(4,5)=3600, &END
 &D SPEC(5,1)=2.5,SPEC(9,1)=55000,SPEC(4,5)=3800,SPEC(1,2)=2.0, &END
```

```
TEST CASE:  SEPARATE FLOW TURBOFAN SANFORD NEW
 &D ICEC=1, LONG=F, NCODE=1, DRAW=F, NMODES=1, &END
REACTANTS
N 1.5606   O 0.4198  AR  .0098                     100.      0.0  G 298.15 O
C 0.5245   H 1.0000                                100.  -4628.066L 298.15 F

NAMELIST
 &INPT2 IDBUG=1,&END
END
 &D MODE=1,
 XNUM=4HINLT,4HLPCI,4HSPLI,4HHPCI,4HMBRN,4HHPTI,4HSBRN,4HLPTI,
 4HABRN,4HNOZI,4HNOZO,4HABRN,4HNOZI,4HNOZO,4HBLED,
 KONFIG(1,1)=4HINLT,1,0,2,0,SPEC(1,1)=100.0,0.,0.,0.,0.,0.,0.,
 0.,0.,0.,0.,18.00,
 KONFIG(1,2)=4HCOMP,2,0,3,13,SPEC(1,2)=1.7,.001,1,1001,1,1002,1,
 1003,1,0.,0.,0.85,3.,1.,
 KONFIG(1,3)=4HSPLT,3,0,4,12,SPEC(1,3)=.63,0.02,0.02,
 KONFIG(1,4)=4HCOMP,4,0,5,0,SPEC(1,4)=1.3,0.,1.,1004,1,1005,1,1006,1,0.,0.,
  0.84,6.,1,
 KONFIG(1,5)=4HDUCT,5,0,6,0,SPEC(1,5)=.05,0,0,3200,.99,18300.,
 FARRAY(1,5)=2.,1.,
 KONFIG(1,6)=4HTURB,6,0,7,0,SPEC(1,6)=3.3,0,1,1007,1,1008,1,1,1,1,.90,5000,1,
 KONFIG(1,7)=4HDUCT,7,0,8,0,SPEC(1,7)=.05,0,0,3400.,.99,18300.,
 FARRAY(1,7)=2.,1.,
 KONFIG(1,8)=4HTURB,8,15,9,0,SPEC(1,8)=1.6,1.0,1,1009,1,1010,1,1,1,1,.90,5000,
  1,
 KONFIG(1,9)=4HDUCT,9,0,10,0,SPEC(1,9)=.05,0,0,0.,.99,18300.,
 FARRAY(1,9)=2.,1.,
 KONFIG(1,10)=4HNOZZ,10,0,11,0,SPEC(1,10)=0.,0.98,0.,0.,.98,1.,1.,0.,1.,
 KONFIG(1,11)=4HDUCT,12,0,13,0,SPEC(1,11)=.05,0,0,0,.99,18300.,
 FARRAY(1,11)=2.,1.,
 KONFIG(1,12)=4HNOZZ,13,0,14,0,SPEC(1,12)=0.,0.98,0.,0.,0.98,1.,1.,0.,1.,
 KONFIG(1,13)=4HSHFT,2,8,0,0,SPEC(1,13)=9*1.0,
 KONFIG(1,14)=4HSHFT,4,6,0,0,SPEC(1,14)=9*1.0,
 KONFIG(1,15)=4HCNTL,SPCNTL(1,15)=1,1,4HSTAP,8,2,0,0,
 KONFIG(1,16)=4HCNTL,SPCNTL(1,16)=1,4,4HSTAP,8,4,0,0,
 KONFIG(1,17)=4HCNTL,SPCNTL(1,17)=1,6,4HSTAP,8,6,0,0,
 KONFIG(1,18)=4HCNTL,SPCNTL(1,18)=1,8,4HSTAP,8,8,0,0,
 KONFIG(1,19)=4HCNTL,SPCNTL(1,19)=1,3,4HDOUT,8,13,0,0,
 KONFIG(1,20)=4HCNTL,SPCNTL(1,20)=1,14,4HDOUT,8,14,0,0,
 &END
 &D DRAW=F,SPEC(9,15)=1,SPEC(9,16)=1,SPEC(9,17)=1,SPEC(9,18)=1,SPEC(9,19)=1,
 SPEC(9,20)=1,SPEC(5,1)=.26,SPEC(9,1)=50,SPEC(6,1)=0,&END
 &D SPEC(5,1)=.6,SPEC(9,1)=10000,&END
 &D SPEC(5,1)=.9,SPEC(9,1)=25000,&END
 &D SPEC(5,1)=1.2,SPEC(9,1)=32200,&END
 &D SPEC(5,1)=1.5,SPEC(9,1)=39500,&END
 &D SPEC(5,1)=1.8,SPEC(9,1)=46800,&END
 &D SPEC(5,1)=2.0,SPEC(9,1)=50900,&END
 &D SPEC(5,1)=2.5,SPEC(9,1)=55000,&END
 &D SPEC(5,1)=3.0,SPEC(9,1)=58400,&END
```

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TEST CASE:  1-SPOOL TBE   SANFORD NEW
 &D ICEC=1,NCOMP=9,NOSTAT=11,DRAW=T,NCODE=1,LONG=F,AMAC=F, &END
REACTANTS
N 1.5606  O 0.4198  AR .0098                        100.0 M    0.0       G 298.15 O
C 0.5245  H 1.0000                                  100.0 M  -4628.066L 298.15 F

END
 &D MODE=1,
 XNUM=4HINLT,4HHPCI,4HDUCT,4HMBRN,4HHPTI,4HDUCT,4HABRN,4HNOZI,
 4HNOZO,4HBLED,4HBPAS,
 KONFIG(1,1)=4HINLT,1,0,2,0,SPEC(1,1)=0,4*0,0,0,.00001,2*0,0,0,100,
 KONFIG(1,2)=4HCOMP,2,0,3,10,SPEC(1,2)=1.3,.001,1,1004,1,1005,1,1006,1,
 0,0,.84,4,1.0,
 KONFIG(1,3)=4HDUCT,3,0,4,11,SPEC(1,3)=8*0,.15,
 KONFIG(1,4)=4HDUCT,4,0,5,0,SPEC(1,4)=.0616,0,0,3000.,.99,18300.,
 FARRAY(1,4)=2,1,
 KONFIG(1,5)=4HTURB,5,10,6,0,SPEC(1,5)=3.32,1,1,1007,1,1008,1,1,
 .6,.86,.90,5000,1,0,0,
 KONFIG(1,6)=4HDUCT,6,11,7,0,SPEC(1,6)=7*0,1,1,
 KONFIG(1,7)=4HDUCT,7,0,8,0,SPEC(1,7)=3*0,0,.99,18300.,
 FARRAY(1,7)=2,1,
 KONFIG(1,8)=4HNOZZ,8,0,9,0,SPEC(1,8)=0,1,0,0,.985,1,1,0,1,
 KONFIG(1,9)=4HSHFT,2,5,0,0,SPEC(1,9)=1,1,1,0,0,1,1,
 KONFIG(1,10)=4HCNTL,SPCNTL(1,10)=1,2,4HSTAP,8,2,0,0,
 KONFIG(1,11)=4HCNTL,SPCNTL(1,11)=1,5,4HSTAP,8,5,0,0,
 KONFIG(1,12)=4HCNTL,SPCNTL(1,12)=14,1,4HDOUT,8,9,0,0,
 KONFIG(1,13)=4HCNTL,SPCNTL(1,13)=1,9,4HDOUT,5,2,20,0,
 KONFIG(1,14)=4HCNTL,SPCNTL(1,14)=9,3,4HDOUT,5,2,20,0,
 &END
 &D DRAW=F,SPEC(5,1)=.26,SPEC(6,1)=0,SPEC(9,1)=50,
 SPEC(9,10)=1,SPEC(9,11)=1,SPEC(9,12)=1,SPEC(9,14)=1,&END
 &D SPEC(5,1)=.6,SPEC(9,1)=10000,&END
 &D SPEC(5,1)=.9,SPEC(9,1)=25000,&END
 &D SPEC(5,1)=1.2,SPEC(9,1)=32200,&END
 &D SPEC(5,1)=1.5,SPEC(9,1)=39500,&END
 &D SPEC(5,1)=1.8,SPEC(9,1)=46800,&END
 &D SPEC(5,1)=2.0,SPEC(9,1)=50900,SPEC(4,4)=3100, &END
 &D SPEC(5,1)=2.5,SPEC(9,1)=55000,
 SPEC(9,3)=0,SPEC(9,14)=0,&END
 &D SPEC(5,1)=3.0,SPEC(9,1)=58400,&END
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ATR WITH HYDROGEN TO TEST SANFORD'S NEW PROGRAM
 &D LONG=F,DRAW=T,ICEC=1,NCODE=-1,NCOMP=13,NOSTAT=10, &END
REACTANTS
N 1.5606  0 0.4198  AR .0098                     100.0 M   0.0  G 298.15 O
C 1.       H 4.                                  100.0    -21390.L 111.66 F
0 2.                                             100.    -3102. L 90.18  0
C 1.       H 4.                                  100.0    21500.G 298.15BF0.995

END
 &D MODE=1,
 KONFIG(1,1)=4HINLT,1,0,2,0,SPEC(1,1)=100,4*0,.97,2*0,.1,2*0,14
 KONFIG(1,2)=4HCOMP,2,0,3,0,SPEC(1,2)=1.6,0,1,1001,1,1002,1,1003,
 1,0,0,.85,2.0,1.,
 KONFIG(1,3)=4HSPLT,3,0,4,5,SPEC(1,3)=0.,0.,
 KONFIG(1,4)=4HMIXR,4,10,7,0,SPEC(1,4)=0.,0.,0.25,.95,
 KONFIG(1,5)=4HGGEN,5,0,6,0,SPEC(1,5)=2960,.67184,600.,1.644,
 FARRAY(1,5)=2,1,
 OARRAY(1,5)=3,1,
 KONFIG(1,6)=4HDUCT,7,0,8,0,SPEC(1,6)=.05,0,0,-0.058,0.995,21500.,
 FARRAY(1,6)=4,1,
 KONFIG(1,7)=4HNOZZ,8,0,9,0,SPEC(1,7)=0,1,0,0,.985,1,1,0,1,
 KONFIG(1,8)=4HTURB,6,0,10,0,SPEC(1,8)=3.6,0.,1,1007.,1,
 1008,1,1,0,1,.80,5000,1,
 KONFIG(1,9)=4HSHFT,2,8,0,0,SPEC(1,9)=9*1,
 KONFIG(1,10)=4HCNTL,SPCNTL(1,10)=1.0,1.0,4HSTAP,8.0,2.0,0.,.0,0.,0.,
 KONFIG(1,11)=4HCNTL,SPCNTL(1,11)=4.0,5.0,4HDOUT,8.0,4.0,0,0,0.,0.,
 KONFIG(1,12)=4HCNTL,SPCNTL(1,12)=3.0,5.0,4HSTAP,8.0,6.0,0.,.0,0.,0.,
 KONFIG(1,13)=4HCNTL,SPCNTL(1,13)=1.0,8.0,4HDOUT,8.0,9.0,0.,.0,0.,0.,
 KONFIG(1,14)=4HCNTL,SPCNTL(1,14)=1.0,9.0,4HDOUT,5.0,2.0,20.,.0,0.,0.,
 KONFIG(1,15)=4HCNTL,SPCNTL(1,15)=4.0,5.0,4HSTAP,2.0,10.0,28.510,0,0,0,
 XNUM=4HINLT,4HHPCI,4HHPCO,4HMIXP,4HWGAS,4HHPTI,4HMIXO,4HNOZI,
 4HNOZO,4HMIXS,
 &END
 &D DRAW=F,SPEC(9,10)=1,SPEC(9,11)=1,SPEC(9,12)=1,SPEC(9,13)=1,
 SPEC(5,1)=.26,SPEC(9,1)=50,SPEC(6,1)=0,&END
 &D SPEC(5,1)=.6,SPEC(9,1)=10000,&END
 &D SPEC(5,1)=.9,SPEC(9,1)=25000,&END
 &D SPEC(5,1)=1.2,SPEC(9,1)=32200,&END
 &D SPEC(5,1)=1.5,SPEC(9,1)=39500,&END
 &D SPEC(5,1)=1.8,SPEC(9,1)=46800,&END
 &D SPEC(5,1)=2.0,SPEC(9,1)=50900,&END
 &D SPEC(5,1)=2.5,SPEC(9,1)=55000,&END
 &D SPEC(5,1)=3.0,SPEC(9,1)=58400
 SPEC(9,3)=0,SPEC(9,14)=0,&END
 &D SPEC(5,1)=3.0,SPEC(9,1)=58400,&END
```

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TABLE 1 - REACTANTS CARD IMAGE

Order	Contents	Format	Columns
First	REACTANTS	3A4	1 to 9
Any	One card for each reactant species (maximum 24). Each card contains:		
	(1) Atomic symbols and formula numbers (maximum 5 sets)[a]	5(A2,F7.5)	1 to 45
	(2) Enthalpy or heat of combustion[b]	F9.5	54 to 62
	(3) State: S, L, or G for solid, liquid, or gas, respectively	A1	63
	(4) Temperature associated with enthalpy in (2)	F7.5	64 to 70
	(5) Blank, J or B	A1	71
	(6) Combustion efficiency (default is 1.00)	F8.5	73 to 80
Last	Blank		

a. If zeros are put in columns 37 & 38, the program will automatically calculate the enthalpy of the reactant at the specified temperature (4), provided that the same species as the reactant is also in the thermodynamic data set.

b. Enthalpy if column 71 is blank or J (Units are cal/g-mole if blank or J/formula wt. if J). Heat of combustion in BTU/lb if column 71 is B.

Table 2. - Values of ARG and Calculated Parameter in Function THERM

ID	ARG (Independent parameter)	Value Calculated (Dependent parameter)
1	enthalpy, BTU/lb	temperature, °R
2	temperature, °R	relative pressure ratio
3	relative pressure ratio	temperature, °R
4	temperature, °R	enthalpy, BTU/lb
5	temperature, °R	specific heat ratio
6	fuel/air ratio	R/M (universal gas constant/ molecular weight)

Table 3. - Values of ARG and DUMMYP in Subroutine THERME

ID	ARG	DUMMYP
1	enthalpy, BTU/lb	pressure, psi
2*	temperature ratio	pressure, psi
3*	pressure ratio	pressure, psi
4,5,6	temperature, °R	pressure, psi
7*	enthalpy, BTU/lb	(not used)
8*	Mach no. (squared)	(not used)

*Isentropic process. Assumes required values such as entropy and/or pressure have already been stored for initial point.

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13. ABSTRACT (Maximum 200 words)

The Navy/NASA Engine Program—NNEP, is a general computer program for calculating aircraft engine performance. NNEP has been used extensively to calculate the design and off-design (matched) performance of a broad range of turbine engines, ranging from subsonic turboprops to variable cycle engines for supersonic transports. Recently, however, there has been increased interest in applications for which NNEP is not capable of simulating, such as the use of alternate fuels including cryogenic fuels and the inclusion of chemical dissociation effects at high temperatures. To overcome these limitations, NNEP has now been extended by including a general chemical equilibrium method. This permits consideration of any propellant system and the calculation of performance with dissociation effects. The new extended program is referred to as NNEP89.

14. SUBJECT TERMS

Computer programs; Engine performance; Chemical equilibrium; Turbine engines; Performance prediction

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